

Nonequivalent operator representations for Bose-condensed systems

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Abstract

The necessity of accurately taking into account the existence of nonequivalent operator representations, associated with canonical transformations, is discussed. It is demonstrated that Bose systems in the presence of the Bose-Einstein condensate and without it correspond to different Fock spaces, orthogonal to each other. A composite representation for the field operators is constructed, allowing for a self-consistent description of Bose-condensed systems. Equations of motion are derived from the given Hamiltonian, which guarantees the validity of conservation laws and thermodynamic self-consistency. At the same time, the particle spectrum, obtained either from diagonalizing this Hamiltonian or from linearizing the field-operator equations of motion, has no gap. The condition of the condensate existence assures the absence of the gap in the spectrum, irrespectively to the approximation involved. The suggested self-consistent theory is both conserving and gapless.

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1 Introduction

Physics of Bose-condensed systems has received in recent years much consideration, both in experiment and theory. Numerous references on current literature can be found in the review articles [1–5]. The history of works on Bose-Einstein condensation is surveyed in Ref. [6].

The microscopic theory of Bose-condensed systems is based on the Bogolubov ideas, which have been applied to a low-temperature dilute gas in the pioneering papers [7,8] and expounded in detail in the books [9,10]. A key point in the Bogolubov approach is the separation of condensate on the level of the field operators, with replacing the condensate operator by a nonoperator quantity, playing the role of a condensate wave function. This procedure is asymptotically exact in the thermodynamic limit [11]. In general terms, this is formulated as the Bogolubov shift, when the field operator is shifted by the condensate wave function. This approach gives for the dilute Bose gas the famous Bogolubov spectrum having at low momenta the phonon character [7–10]. Beliaev [12,13] included in the Bogolubov approach interactions between quasiparticles, obtaining, by means of perturbation theory at zero temperature, attenuation parameters. Hugenholtz and Pines [14] formulated the condition on the chemical potential, providing a gapless quasiparticle spectrum at zero temperature. This condition was generalized to finite temperatures by Bogolubov [9,10] and Hohenberg and Martin [15]. The Beliaev zero-temperature calculations were extended to finite temperatures by Popov and Faddeev [16] and Popov [17–19]. The Bogolubov theory was applied to inhomogeneous systems by Fetter [20]. The Beliaev-Popov approach was extended to nonuniform trapped gases by Fedichev and Shlyapnikov [21] and by Morgan et al. [22–25].

In the lowest dilute-gas approximations, such as the Bogolubov and Beliaev-Popov approximations, the quasiparticle spectrum is gapless, in agreement with the Goldstone and Bogolubov theorems [9,10,15]. However, in higher approximations, the spectrum acquires a nonphysical gap, which happens, e.g., in the Hartree-Fock-Bogolubov approximation. The standard remedy for removing the gap is to construct higher-order vertex equations, such as the Bethe-Salpeter equation or Lipmann-Schwinger equation, including additional terms into the theory in order to compensate the gap [26]. But so constructed compensations are not a result of a self-consistent scheme, in which all equations would follow from one generally prescribed procedure. As a consequence, the resulting modifications suffer from violating conservations laws and thermodynamic consistency. In order to preserve conservation laws, all equations in the theory must be derivable from a given Hamiltonian or some variational functional [27,28]. For one chosen approximation, it is always possible to construct an artificial variational functional that would yield a gapless spectrum and even preserving conservation laws [29,30]. However, this cannot be considered as a self-consistent theory allowing for a systematic derivation of other approximations. In this way, all theories of Bose-condensed systems suffer either from the absence of conservation laws and thermodynamic consistency or from the presence of an unphysical gap in the quasiparticle spectrum. A detailed classification of theories onto either conserving but gapless or gapless but nonconserving has been done by Hohenberg and Martin [15].

The aim of the present paper is to suggest a self-consistent theory that would be both conserving as well as gapless. To be conserving, the theory must be based on one mi-

microscopic Hamiltonian, from which all equations would follow. To be gapless, the theory requires an accurate mathematical formulation, taking account of the existence of the Bose-condensed fraction. Such an accurate mathematical formulation can be done by explicitly taking into consideration the appearance of nonequivalent operator representations associated with canonical commutation relations [31]. Since the theory to be developed rests on the notion of nonequivalent operator representations, it is necessary, first of all, to specify its meaning for Bose-condensed systems, which is done in Sections 2 and 3. Then, in Section 4, a composite representation is defined, making it possible to accurately describe Bose-condensed systems. Equations of motion are derived in Section 5 from a microscopic Hamiltonian based on the composite representation. To make the resulting equations more transparent, they are illustrated for the case of a uniform dilute gas in Section 6. The generalization to nonuniform matter is given in Section 7. Everywhere the system of units is employed, where the Planck constant $\hbar = 1$ and the Boltzmann constant $k_B = 1$ are set to unity. The material of this paper is based on the Lectures [32].

2 Bogolubov shift

The Bogolubov shift of the field operator is commonly defined as

$$\psi(\mathbf{r}, t) = \eta(\mathbf{r}, t) + \psi_1(\mathbf{r}, t) , \quad (1)$$

where $\psi(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$ satisfy the Bose commutation relations and $\eta(\mathbf{r}, t)$ is a condensate wave function, assumed to be not an identical zero. In what follows, for the sake of brevity, the time dependence often will not be shown explicitly, so that we shall write $\psi(\mathbf{r})$, $\eta(\mathbf{r})$, and $\psi_1(\mathbf{r})$, though keeping in mind that, in general, these quantities do depend on time.

Field operators act on functions pertaining to a Fock space. Let the field operators $\psi(\mathbf{r})$ and $\psi^\dagger(\mathbf{r})$ be defined on the corresponding Fock space $\mathcal{F}(\psi)$. Let $|0\rangle$ be the vacuum state of $\mathcal{F}(\psi)$, such that for any \mathbf{r} one has

$$\psi(\mathbf{r})|0\rangle = 0 . \quad (2)$$

Then any function $\varphi \in \mathcal{F}(\psi)$ can be generated by a repeated action of $\psi^\dagger(\mathbf{r})$ according to the rule

$$\varphi = \sum_{n=0}^{\infty} \frac{1}{\sqrt{n!}} \int f_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \prod_{i=1}^n \psi^\dagger(\mathbf{r}_i) d\mathbf{r}_i |0\rangle .$$

In that sense, one says that the Fock space $\mathcal{F}(\psi)$ is generated by $\psi^\dagger(\mathbf{r})$.

It is easy to notice that the state $|0\rangle$ is not a vacuum for $\psi_1(\mathbf{r})$, since

$$\psi_1(\mathbf{r})|0\rangle = -\eta(\mathbf{r})|0\rangle \neq 0 . \quad (3)$$

A vacuum for $\psi_1(\mathbf{r})$ is another state, which will be denoted as $|0\rangle_1$, and which satisfies the vacuum-state equation

$$\psi_1(\mathbf{r})|0\rangle_1 = 0 . \quad (4)$$

In line with the general rules [33], the creation operator $\psi_1^\dagger(\mathbf{r})$ generates the Fock space $\mathcal{F}(\psi_1)$. Clearly, the vacuum state $|0\rangle_1$ is not a vacuum for $\psi(\mathbf{r})$, as far as

$$\psi(\mathbf{r})|0\rangle_1 = \eta(\mathbf{r})|0\rangle_1 \neq 0 . \quad (5)$$

Thus, transformation (1) cannot be understood as an operator equality defined on one Fock space.

Let us introduce the operator

$$\hat{C} \equiv \exp \left\{ \int \left[\eta^*(\mathbf{r})\psi(\mathbf{r}) - \eta(\mathbf{r})\psi^\dagger(\mathbf{r}) \right] d\mathbf{r} \right\} \quad (6)$$

and its inverse

$$\hat{C}^{-1} = \exp \left\{ - \int \left[\eta^*(\mathbf{r})\psi(\mathbf{r}) - \eta(\mathbf{r})\psi^\dagger(\mathbf{r}) \right] d\mathbf{r} \right\} . \quad (7)$$

With the help of these operators, relation (1) takes the form

$$\psi(\mathbf{r}) = \hat{C}\psi_1(\mathbf{r})\hat{C}^{-1} \quad (8)$$

and, conversely,

$$\psi_1(\mathbf{r}) = \hat{C}^{-1}\psi(\mathbf{r})\hat{C} . \quad (9)$$

By this definition, the operator \hat{C} transforms functions from $\mathcal{F}(\psi_1)$ into those in $\mathcal{F}(\psi)$, while \hat{C}^{-1} transforms the states of $\mathcal{F}(\psi)$ into those of $\mathcal{F}(\psi_1)$. In particular, the relation between the vacua in $\mathcal{F}(\psi)$ and in $\mathcal{F}(\psi_1)$ is

$$|0 >_1 = \hat{C}^{-1}|0 > , \quad (10)$$

which is obvious from Eq. (9).

To better understand the connection between the spaces $\mathcal{F}(\psi)$ and $\mathcal{F}(\psi_1)$, we can use the Baker-Hausdorff formula for any two operators \hat{A} and \hat{B} , whose commutator $[\hat{A}, \hat{B}]$ is proportional to a unity operator. Then

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}} \exp \left(- \frac{1}{2} [\hat{A}, \hat{B}] \right) .$$

Using this formula, operator (7) can be represented as

$$\hat{C}^{-1} = \exp \left\{ \int \eta(\mathbf{r})\psi^\dagger(\mathbf{r}) d\mathbf{r} \right\} \exp \left\{ - \int \eta^*(\mathbf{r})\psi(\mathbf{r}) d\mathbf{r} \right\} \exp \left\{ - \frac{1}{2} \int |\eta(\mathbf{r})|^2 d\mathbf{r} \right\} . \quad (11)$$

Form here, we have

$$\hat{C}^{-1}|0 > = \exp \left\{ - \frac{1}{2} \int |\eta(\mathbf{r})|^2 d\mathbf{r} \right\} \exp \left\{ \int \eta(\mathbf{r})\psi^\dagger(\mathbf{r}) d\mathbf{r} \right\} |0 > . \quad (12)$$

The right-hand side of Eq. (12) is nothing but the coherent state

$$|\eta > = \eta_0 \exp \left\{ \int \eta(\mathbf{r})\psi^\dagger(\mathbf{r}) d\mathbf{r} \right\} |0 > ,$$

normalized to unity, so that

$$|\eta_0| = \exp \left\{ - \frac{1}{2} \int |\eta(\mathbf{r})|^2 d\mathbf{r} \right\} .$$

By definition, the coherent state is given by the eigenproblem

$$\psi(\mathbf{r})|\eta\rangle = \eta(\mathbf{r})|\eta\rangle, \quad (13)$$

whose eigenvalue is a coherent field $\eta(\mathbf{r})$. Hence, vacuum (10) is the coherent state,

$$|0\rangle_1 = \hat{C}^{-1}|0\rangle = |\eta\rangle, \quad (14)$$

and the condensate wave function in the Bogolubov shift (1) is nothing but the coherent field

$$\eta(\mathbf{r}) = \langle \eta | \psi(\mathbf{r}) | \eta \rangle. \quad (15)$$

The scalar product of the vacua $|0\rangle$ and $|0\rangle_1$ is

$$\langle 0 | 0 \rangle_1 = \langle 0 | \eta \rangle = \exp \left\{ -\frac{1}{2} \int |\eta(\mathbf{r})|^2 d\mathbf{r} \right\}, \quad (16)$$

as far as

$$\langle 0 | \exp \left\{ \int \eta(\mathbf{r}) \psi^\dagger(\mathbf{r}) d\mathbf{r} \right\} | 0 \rangle = 1.$$

The condensate wave function defines the condensate density

$$\rho_0(\mathbf{r}) = |\eta(\mathbf{r})|^2. \quad (17)$$

Respectively, the latter determines the number of condensed particles

$$N_0 = \int \rho_0(\mathbf{r}) d\mathbf{r}. \quad (18)$$

So, the scalar product (16) gives

$$\langle 0 | \eta \rangle = \exp \left(-\frac{1}{2} N_0 \right). \quad (19)$$

Bose-Einstein condensation implies that the number of condensed particles N_0 is large, being of the order of the total number of particles N . Therefore product (19) is asymptotically zero,

$$\langle 0 | \eta \rangle \simeq 0 \quad (N_0 \gg 1).$$

That is, the vacua $|0\rangle$ and $|0\rangle_1$ are asymptotically orthogonal. Similarly, all states generated by $\psi^\dagger(\mathbf{r})$ from $|0\rangle$ are orthogonal to the states generated by $\psi_1^\dagger(\mathbf{r})$ from $|0\rangle_1$. This is equivalent to saying that the Fock spaces $\mathcal{F}(\psi)$ and $\mathcal{F}(\psi_1)$ are asymptotically orthogonal to each other. There is the sole state that is shared by both these spaces. This is the coherent state $|\eta\rangle$ of $\mathcal{F}(\psi)$, which is at the same time the vacuum $|0\rangle_1 = |\eta\rangle$ of $\mathcal{F}(\psi_1)$. But since the spaces $\mathcal{F}(\psi)$ and $\mathcal{F}(\psi_1)$ are of continuous power, the sole intersection is called to be of zero measure.

The operator transformation (6), from $\mathcal{F}(\psi_1)$ to $\mathcal{F}(\psi)$, is not unitary. The inverse transformation (7), from $\mathcal{F}(\psi)$ to $\mathcal{F}(\psi_1)$, is not the same as \hat{C}^+ , since it is not defined in one space. To be unitary, an operator and its Hermitian conjugate must be defined in one space. Therefore the Bogolubov shift (1) realizes the unitary nonequivalent representations of the field operators satisfying the Bose commutation relations. Strictly speaking, Eq. (1) has

no sense of an operator equation, since its left-hand and right-hand sides are defined on different Fock spaces orthogonal to each other. More correctly, it has to be interpreted not as an equation but as a replacement

$$\psi(\mathbf{r}) \longrightarrow \eta(\mathbf{r}) + \psi_1(\mathbf{r}) , \quad (20)$$

with its left-hand side being defined on $\mathcal{F}(\psi)$ and the right-hand side, on $\mathcal{F}(\psi_1)$.

As a physical interpretation, we may say that the field operator $\psi(\mathbf{r})$ describes the Bose system *before* Bose-Einstein condensation has occurred, while the operator $\eta(\mathbf{r}) + \psi_1(\mathbf{r})$ corresponds to that Bose system *after* the occurrence of Bose-Einstein condensation. This is somewhat analogous to the Van Hove picture of scattering [34,35], according to which the particle states, before the scattering process has occurred, are orthogonal to their states after the scattering. That is, the Fock space of particles before the scattering is orthogonal to their Fock space after the scattering. Thence the particle field operators before and after the scattering process pertain to unitary nonequivalent representations of the same commutation relations.

It is important to emphasize that the right-hand side of replacement (20) clearly breaks the gauge symmetry. The latter could also be broken in the space $\mathcal{F}(\psi)$ by adding to the Hamiltonian infinitesimal sources breaking this symmetry. However, irrespectively to whether the gauge symmetry in $\mathcal{F}(\psi)$ is broken or not, this space remains always orthogonal to $\mathcal{F}(\psi_1)$. This means that by breaking in $\mathcal{F}(\psi)$ the gauge symmetry solely by infinitesimal sources (without the Bogolubov shift) one cannot make the transformation from $\mathcal{F}(\psi)$ to $\mathcal{F}(\psi_1)$. For the correct description of a Bose-condensed system it is not sufficient just to add to a Hamiltonian infinitesimal sources breaking the gauge symmetry, but it is necessary to make the Bogolubov shift, transferring the consideration to another space. Recall that separating in the Hamiltonian the condensate field operators is equivalent to the Bogolubov shift, because the condensate operators, under the thermodynamic limit, become nonoperator quantities representing the condensate wave function [9–11].

3 Canonical transformations

The Bogolubov shift (1) or (20) is an example of a simple canonical transformation realizing unitary nonequivalent operator representations. Another canonical transformation, constantly employed in the theory of Bose systems, is the Bogolubov canonical transformation

$$a_k = u_k b_k + v_{-k}^* b_{-k}^\dagger \quad (21)$$

from the operators a_k and a_k^\dagger to b_k and b_k^\dagger , where the label k implies a set of quantum numbers, e.g., the momentum. The inverse transformation is

$$b_k = u_k^* a_k - v_k^* a_{-k}^\dagger . \quad (22)$$

In order that a_k and b_k would satisfy the same Bose commutation relations, the coefficient functions have to obey the normalization condition

$$|u_k|^2 - |v_k|^2 = 1 .$$

Transformations (21) and (22) also realize unitary nonequivalent operator representations. Showing this below, we shall explain how this case differs from that considered in the previous section.

Let $|0 \rangle_a$ be the vacuum state for the operator a_k , so that

$$a_k |0 \rangle_a = 0 . \quad (23)$$

Using the standard procedure [33], one can construct the Fock space $\mathcal{F}(a_k)$ generated by a_k^\dagger . The state $|0 \rangle_a$ is not a vacuum for b_k , since

$$b_k |0 \rangle_a = -v_k^* a_{-k}^\dagger |0 \rangle_a \neq 0 .$$

The operators b_k possess another vacuum $|0 \rangle_b$, for which

$$b_k |0 \rangle_b = 0 . \quad (24)$$

And $|0 \rangle_b$ is not a vacuum for a_k , because

$$a_k |0 \rangle_b = v_{-k}^* b_{-k}^\dagger |0 \rangle_b \neq 0 .$$

The Fock space $\mathcal{F}(b_k)$ is generated by b_k^\dagger .

Usually, the coefficient functions can be chosen to be real and invariant under the change of k onto $-k$, which we shall assume below setting

$$u_k^* = u_{-k} = u_k , \quad v_k^* = v_{-k} = v_k .$$

Introducing the quantity

$$\alpha_k \equiv \ln(u_k + v_k) , \quad (25)$$

one may write

$$u_k = \cosh \alpha_k , \quad v_k = \sinh \alpha_k . \quad (26)$$

Define the operator

$$\hat{B} \equiv \exp \left\{ \frac{1}{2} \sum_k \alpha_k \left(a_k a_{-k} - a_{-k}^\dagger a_k^\dagger \right) \right\} \quad (27)$$

and its inverse

$$\hat{B}^{-1} = \exp \left\{ -\frac{1}{2} \sum_k \alpha_k \left(a_k a_{-k} - a_{-k}^\dagger a_k^\dagger \right) \right\} . \quad (28)$$

Using this, transformations (21) and (22) can be represented as

$$a_k = \hat{B} b_k \hat{B}^{-1} \quad (29)$$

and, respectively, as

$$b_k = \hat{B}^{-1} a_k \hat{B} . \quad (30)$$

The operator \hat{B} transforms $\mathcal{F}(b_k)$ into $\mathcal{F}(a_k)$, while \hat{B}^{-1} transforms $\mathcal{F}(a_k)$ into $\mathcal{F}(b_k)$. Thus, the vacua in these spaces are related by the transformation

$$|0 \rangle_b = \hat{B}^{-1} |0 \rangle_a . \quad (31)$$

Involving the Baker-Hausdorff formula, we can represent operator (28) as

$$\hat{B}^{-1} = \exp \left(\frac{1}{2} \sum_k \alpha_k a_{-k}^\dagger a_k^\dagger \right) \exp \left(-\frac{1}{2} \sum_k \alpha_k a_k a_{-k} \right) \exp \left\{ -\frac{1}{4} \sum_k \alpha_k^2 (1 + 2a_k^\dagger a_k) \right\}, \quad (32)$$

keeping in mind its action on vacuum $|0\rangle_a$, for which

$$\sum_{kp} \alpha_k \alpha_p [a_{-k}^\dagger a_k^\dagger, a_p a_{-p}] |0\rangle_a = \sum_k \alpha_k^2 (1 + 2a_k^\dagger a_k) |0\rangle_a = \sum_k \alpha_k^2 |0\rangle_a.$$

Then for vacuum (31), we find

$$|0\rangle_b = \hat{B}^{-1} |0\rangle_a = \exp \left(-\frac{1}{4} \sum_k \alpha_k^2 \right) \exp \left(\frac{1}{2} \sum_k \alpha_k a_{-k}^\dagger a_k^\dagger \right) |0\rangle_a. \quad (33)$$

The scalar product of the vacua $|0\rangle_a$ and $|0\rangle_b$ is

$${}_a \langle 0 | 0 \rangle_b = \exp \left\{ -\frac{V}{4} \int \alpha_k^2 \frac{d\mathbf{k}}{(2\pi)^3} \right\}, \quad (34)$$

where V is the system volume, and the equality

$${}_a \langle 0 | \exp \left(\frac{1}{2} \sum_k a_{-k}^\dagger a_k^\dagger \right) | 0 \rangle_a = 1$$

is taken into account. The integral in Eq. (34) is positive. As is evident, the vacua are asymptotically orthogonal, so that

$${}_a \langle 0 | 0 \rangle_b \simeq 0 \quad (V \rightarrow \infty).$$

The Fock spaces $\mathcal{F}(a_k)$ and $\mathcal{F}(b_k)$ are mutually orthogonal in the thermodynamic limit. The operator \hat{B} is not unitary. Thus, the canonical transformations (21) and (22) realize unitary nonequivalent operator representations. Since the left-hand and right-hand sides of Eq. (21) are defined on different Fock spaces, it should be understood not as a straightforward operator equality, but as a replacement

$$a_k \longrightarrow u_k b_k + v_{-k}^* b_{-k}^\dagger. \quad (35)$$

The main physical difference between the transformations (20) and (35) is that the latter is not related to the existence or absence of Bose-Einstein condensate, while the Bogolubov shift (2) transforms a system without Bose condensate to a Bose-condensed system.

4 Composite representation

The description of a Bose system without Bose-Einstein condensate can be done in terms of one field operator $\psi(\mathbf{r})$ defined on the Fock space $\mathcal{F}(\psi)$ generated by $\psi^\dagger(\mathbf{r})$ from a vacuum state $|0\rangle$. But a Bose-condensed system requires to employ two variables, the condensate wave function $\eta(\mathbf{r})$ and the operator of noncondensed particles $\psi_1(\mathbf{r})$ defined on the Fock

space $\mathcal{F}(\psi_1)$ generated by $\psi_1^\dagger(\mathbf{r})$ from the vacuum $|0\rangle_1$. In order to stress that there are two variables for a Bose-condensed system, it is possible to treat both condensed and noncondensed particles on an equal footing by introducing a composite representation for the field operators.

As is shown above, the condensate corresponds to the coherent state. We may define the one-dimensional space

$$\mathcal{F}_0 \equiv \{|\eta\rangle\} \quad (36)$$

containing the coherent state for a field operator $\psi_0(\mathbf{r})$, for which

$$\psi_0(\mathbf{r})|\eta\rangle = \eta(\mathbf{r})|\eta\rangle. \quad (37)$$

The operator of noncondensed particles $\psi_1(\mathbf{r})$ is defined on the Fock space $\mathcal{F}(\psi_1)$ generated by $\psi_1^\dagger(\mathbf{r})$ from the vacuum $|0\rangle_1$. In order to avoid the double counting of the degrees of freedom, the orthogonality condition

$$\int \eta^*(\mathbf{r})\psi_1(\mathbf{r}) d\mathbf{r} = 0 \quad (38)$$

is imposed.

Since in the space $\mathcal{F}(\psi_1)$ the gauge symmetry is explicitly broken, the statistical average $\langle \psi_1(\mathbf{r}) \rangle_{\mathcal{F}(\psi_1)}$ over this space may be not zero. This, however, would result in the nonconservation of quantum numbers. For instance, in the case of particles with nonzero spin, the latter would not be conserved. Or, Fourier transforming $\psi_1(\mathbf{r})$ to a_k , and having a nonzero statistical average $\langle a_k \rangle_{\mathcal{F}(a_k)}$, one would confront the absence of momentum conservation. To eliminate such unpleasant features, one defines the restricted space $\mathcal{F}_1 \subset \mathcal{F}(\psi_1)$, such that the restricted average

$$\langle \psi_1(\mathbf{r}) \rangle_{\mathcal{F}_1} = 0 \quad (39)$$

be zero. Formally, the restricted space is defined as

$$\mathcal{F}_1 \equiv \{\varphi \in \mathcal{F}(\psi_1) \mid \langle \psi_1(\mathbf{r}) \rangle_{\mathcal{F}_1} = 0\}. \quad (40)$$

An explicit and mathematically correct definition of the restricted space (40) can be done in terms of the weighted Hilbert spaces [36,37].

Let us now introduce the *composite Fock space*

$$\tilde{\mathcal{F}} \equiv \mathcal{F}_0 \otimes \mathcal{F}_1, \quad (41)$$

being a tensor product of the spaces (36) and (40). And let us define the *composite field operator*

$$\tilde{\psi}(\mathbf{r}) \equiv \psi_0(\mathbf{r}) \oplus \psi_1(\mathbf{r}) \quad (42)$$

acting on the composite space (41). In what follows, we shall simplify the notation often writing, instead of the sign of the direct summation \oplus , just the usual signs of summation or subtraction. We shall also omit, as is usually done, the unity operators $\hat{1}_0$ and $\hat{1}_1$ defined in the corresponding spaces \mathcal{F}_0 and \mathcal{F}_1 .

The condensate wave function, according to definition (37), is the coherent field

$$\eta(\mathbf{r}) = \langle \eta | \psi_0(\mathbf{r}) | \eta \rangle. \quad (43)$$

The number-of-particle operator of condensed particles, defined in the space \mathcal{F}_0 , is

$$\hat{N}_0 \equiv \int \psi_0^\dagger(\mathbf{r}) \psi_0(\mathbf{r}) d\mathbf{r} . \quad (44)$$

The condensate wave function is normalized to the number of condensed particles

$$N_0 \equiv \langle \eta | \hat{N}_0 | \eta \rangle = \int |\eta(\mathbf{r})|^2 d\mathbf{r} . \quad (45)$$

The vectors $f \in \tilde{\mathcal{F}}$, pertaining to the composite space (41), have the structure of the tensor product

$$f = |\eta\rangle \otimes \varphi ,$$

in which $|\eta\rangle \in \mathcal{F}_0$ and $\varphi \in \mathcal{F}_1$. For any two vectors $f_m, f_n \in \tilde{\mathcal{F}}$, the matrix element of the composite field operator (42) is

$$f_m^+ \tilde{\psi}(\mathbf{r}) f_n = \varphi_m^+ \langle \eta | \tilde{\psi}(\mathbf{r}) | \eta \rangle \varphi_n = \varphi_m^+ [\eta(\mathbf{r}) + \psi_1(\mathbf{r})] \varphi_n . \quad (46)$$

Respectively, the matrix element of an operator $\hat{A}[\tilde{\psi}]$ from the algebra of local observables on $\tilde{\mathcal{F}}$ takes the form

$$f_m^+ \hat{A}[\tilde{\psi}] f_n = \varphi_m^+ \langle \eta | \hat{A}[\tilde{\psi}] | \eta \rangle \varphi_n = \varphi_m^+ \hat{A}[\eta + \psi_1] \varphi_n . \quad (47)$$

The trace of such an operator is

$$\text{Tr}_{\tilde{\mathcal{F}}} \hat{A}[\tilde{\psi}] = \text{Tr}_{\mathcal{F}_1} \langle \eta | \hat{A}[\tilde{\psi}] | \eta \rangle = \text{Tr}_{\mathcal{F}_1} \hat{A}[\eta + \psi_1] .$$

The statistical average over the space $\tilde{\mathcal{F}}$, with respect to a statistical operator $\hat{\rho}[\tilde{\psi}]$, taken at the initial time $t = 0$, writes as

$$\langle \hat{A}[\tilde{\psi}] \rangle_{\tilde{\mathcal{F}}} \equiv \text{Tr}_{\tilde{\mathcal{F}}} \hat{\rho}[\tilde{\psi}] \hat{A}[\tilde{\psi}] = \text{Tr}_{\mathcal{F}_1} \hat{\rho}[\eta + \psi_1] \hat{A}[\eta + \psi_1] . \quad (48)$$

Defining the average over \mathcal{F}_1 as

$$\langle \hat{A}[\eta + \psi_1] \rangle_{\mathcal{F}_1} \equiv \text{Tr}_{\mathcal{F}_1} \hat{\rho}[\eta + \psi_1] \hat{A}[\eta + \psi_1] , \quad (49)$$

we get

$$\langle \hat{A}[\tilde{\psi}] \rangle_{\tilde{\mathcal{F}}} = \langle \hat{A}[\eta + \psi_1] \rangle_{\mathcal{F}_1} . \quad (50)$$

The operator of the total number of particles

$$\hat{N} \equiv \int \tilde{\psi}^\dagger(\mathbf{r}) \tilde{\psi}(\mathbf{r}) d\mathbf{r} , \quad (51)$$

with the composite field operator (42), keeping in mind the orthogonality condition (38), can be represented as the direct sum

$$\hat{N} = \hat{N}_0 \oplus \hat{N}_1 \quad (52)$$

of the condensed-particle operator (44) and the operator for the number of noncondensed particles

$$\hat{N}_1 \equiv \int \psi_1^\dagger(\mathbf{r}) \psi_1(\mathbf{r}) d\mathbf{r} . \quad (53)$$

The average of the total number-of-particle operator (51), according to Eq. (50), becomes

$$\langle \hat{N} \rangle_{\tilde{\mathcal{F}}} = N_0 + \langle \hat{N}_1 \rangle_{\mathcal{F}_1} . \quad (54)$$

The equality

$$N = \langle \hat{N} \rangle_{\tilde{\mathcal{F}}} \quad (55)$$

for the total number of particles serves as a normalization condition, additional to the normalization (45) for the number of condensed particles. Both these normalization conditions, (45) and (55), must be taken into account in a self-consistent theory.

5 Equations of motion

The energy operator is given by the Hamiltonian

$$\hat{H} = \int \tilde{\psi}^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U \right) \tilde{\psi}(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \tilde{\psi}^\dagger(\mathbf{r}) \tilde{\psi}^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \tilde{\psi}(\mathbf{r}') \tilde{\psi}(\mathbf{r}) d\mathbf{r} d\mathbf{r}' , \quad (56)$$

in which, m is particle mass, $U = U(\mathbf{r}, t)$ is an external field, and $\Phi(\mathbf{r}) = \Phi(-\mathbf{r})$ is an interaction potential, assumed to be integrable, so that

$$\left| \int_V \Phi(\mathbf{r}) d\mathbf{r} \right| < \infty .$$

The field operators $\tilde{\psi}(\mathbf{r}) = \tilde{\psi}(\mathbf{r}, t)$ are given in the Heisenberg representation, but the temporal variable t is not explicitly shown just for making the formulas less cumbersome.

To take into consideration two normalization conditions, (45) and (55), it is necessary to introduce two Lagrange multipliers, μ_0 and μ , entering the grand Hamiltonian

$$H[\tilde{\psi}] = \hat{H} - \mu_0 \hat{N}_0 - \mu \hat{N} . \quad (57)$$

Here μ is the conventional chemical potential and μ_0 is an additional Lagrange multiplier guaranteeing the validity of the normalization condition (45).

With the composite field operator (42), the Hamiltonian (57) can be represented as a sum

$$H[\tilde{\psi}] = \sum_{n=0}^4 H^{(n)} , \quad (58)$$

in which the terms are classified according to the number of the noncondensed-particle operators in the products of each term. Thus, the zero-order term contains only the condensate field operators,

$$\begin{aligned} H^{(0)} = & \int \psi_0^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U - \mu_0 - \mu \right) \psi_0(\mathbf{r}) d\mathbf{r} + \\ & + \frac{1}{2} \int \psi_0^\dagger(\mathbf{r}) \psi_0^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \psi_0(\mathbf{r}') \psi_0(\mathbf{r}) d\mathbf{r} d\mathbf{r}' . \end{aligned} \quad (59)$$

The first-order term is

$$H^{(1)} = \int \psi_1^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_0(\mathbf{r}) d\mathbf{r} + \int \psi_1(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_0^\dagger(\mathbf{r}) d\mathbf{r} +$$

$$+ \int \Phi(\mathbf{r} - \mathbf{r}') \left[\psi_1^\dagger(\mathbf{r}) \psi_0^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_0(\mathbf{r}) + \psi_0^\dagger(\mathbf{r}) \psi_0^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_1(\mathbf{r}) \right] d\mathbf{r} d\mathbf{r}' . \quad (60)$$

However, a Hamiltonian term of the first order in $\psi_1(\mathbf{r})$ or $\psi_1^\dagger(\mathbf{r})$, being considered on the space \mathcal{F}_1 defined in Eq. (40), is effectively zero due to the conservation condition (39). If a Hamiltonian would contain such linear in $\psi_1(\mathbf{r})$ or $\psi_1^\dagger(\mathbf{r})$ terms, condition (39) could not be satisfied. The same can be said in another manner. To take into account restriction (39), we could add to the grand Hamiltonian (57) one more term with a Lagrange multiplier assuring the validity of Eq. (39). To this end, this additional term has to be chosen so that to cancel the linear term (60). In any way,

$$H^{(1)} = 0 . \quad (61)$$

For the quadratic term in Eq. (58), we have

$$\begin{aligned} H^{(2)} = & \int \psi_1^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_1(\mathbf{r}) d\mathbf{r} + \\ & + \int \Phi(\mathbf{r} - \mathbf{r}') \left[\psi_0^\dagger(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_0(\mathbf{r}) + \psi_0^\dagger(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_1(\mathbf{r}) + \right. \\ & \left. + \frac{1}{2} \psi_0^\dagger(\mathbf{r}) \psi_0^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \frac{1}{2} \psi_1^\dagger(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_0(\mathbf{r}) \right] d\mathbf{r} d\mathbf{r}' . \end{aligned} \quad (62)$$

The third-order term is

$$H^{(3)} = \int \Phi(\mathbf{r} - \mathbf{r}') \left[\psi_0^\dagger(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_0(\mathbf{r}) \right] d\mathbf{r} d\mathbf{r}' . \quad (63)$$

In expressions (62) and (63), the symmetry $\Phi(\mathbf{r}) = \Phi(-\mathbf{r})$ is used. The last term is

$$H^{(4)} = \frac{1}{2} \int \psi_1^\dagger(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) d\mathbf{r} d\mathbf{r}' . \quad (64)$$

In order to preserve all conservation laws, such as the continuity equation, the density of current, and the energy-momentum conservation laws, all equations of motion must be derived from the same Hamiltonian. A theory with such Hamiltonian-derivable equations will automatically be conserving. Since we have two field-operator variables, we should have two types of equations of motion.

The first equation prescribes the evolution of the condensate operator

$$i \frac{\partial}{\partial t} \psi_0(\mathbf{r}, t) = \frac{\delta H[\psi_0 \oplus \psi_1]}{\delta \psi_0^\dagger(\mathbf{r}, t)} . \quad (65)$$

For the Hamiltonian (58), one has

$$\frac{\delta H[\psi_0 \oplus \psi_1]}{\delta \psi_0^\dagger(\mathbf{r}, t)} = \frac{\delta}{\delta \psi_0^\dagger(\mathbf{r}, t)} \left(H^{(0)} + H^{(2)} + H^{(3)} \right) .$$

In the expressions below, we shall again write $\psi_0(\mathbf{r})$ and $\psi_1(\mathbf{r})$, omitting the time variable in order to simplify the formulas. Then we find the variational derivatives of the zero-order term,

$$\frac{\delta H^{(0)}}{\delta \psi_0^\dagger(\mathbf{r}, t)} = \left(-\frac{\nabla^2}{2m} + U - \mu_0 - \mu \right) \psi_0(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \psi_0^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_0(\mathbf{r}) d\mathbf{r}' ,$$

of the second-order term,

$$\frac{\delta H^{(2)}}{\delta \psi_0^\dagger(\mathbf{r}, t)} = \int \Phi(\mathbf{r} - \mathbf{r}') \left[\psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_0(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_0^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \right] d\mathbf{r}' ,$$

and of the third-order term

$$\frac{\delta H^{(3)}}{\delta \psi_0^\dagger(\mathbf{r}, t)} = \int \Phi(\mathbf{r} - \mathbf{r}') \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) d\mathbf{r}' .$$

Substituting this into Eq. (65) and taking its coherent average yields

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + U - \mu_0 - \mu \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[|\eta(\mathbf{r}')|^2 \eta(\mathbf{r}) + \hat{X}(\mathbf{r}, \mathbf{r}') \right] d\mathbf{r}' , \quad (66)$$

where

$$\hat{X}(\mathbf{r}, \mathbf{r}') \equiv \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \eta(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \eta(\mathbf{r}') \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) . \quad (67)$$

We may note that Eq. (66) can also be derived from the equation

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \frac{\delta H[\eta + \psi_1]}{\delta \eta^*(\mathbf{r}, t)} , \quad (68)$$

which follows from taking the coherent average of Eq. (65).

The second equation of motion describes the evolution of the field operator of noncondensed particles,

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta H[\psi_0 \oplus \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} . \quad (69)$$

With the Hamiltonian (58), we get

$$\frac{\delta H[\psi_0 \oplus \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} = \frac{\delta}{\delta \psi_1^\dagger(\mathbf{r}, t)} \left(H^{(2)} + H^{(3)} + H^{(4)} \right) .$$

The corresponding variational derivatives give for the second-order term

$$\begin{aligned} \frac{\delta H^{(2)}}{\delta \psi_1^\dagger(\mathbf{r}, t)} &= \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_1(\mathbf{r}) + \\ &+ \int \Phi(\mathbf{r} - \mathbf{r}') \left[\psi_0^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_0^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_0(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_0(\mathbf{r}) \right] d\mathbf{r}' , \end{aligned}$$

for the third-order term,

$$\frac{\delta H^{(3)}}{\delta \psi_1^\dagger(\mathbf{r}, t)} = \int \Phi(\mathbf{r} - \mathbf{r}') \left[\psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_0(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \psi_0(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_0^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \right] d\mathbf{r}' ,$$

and for the fourth-order term,

$$\frac{\delta H^{(4)}}{\delta \psi_1^\dagger(\mathbf{r}, t)} = \int \Phi(\mathbf{r} - \mathbf{r}') \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) d\mathbf{r}' .$$

Taking the coherent average of Eq. (69), we obtain

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_1(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[|\eta(\mathbf{r}')|^2 \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}') \psi_1(\mathbf{r}') \eta(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \eta(\mathbf{r}') \eta(\mathbf{r}) + \hat{X}(\mathbf{r}, \mathbf{r}') \right] d\mathbf{r}' . \quad (70)$$

The latter equation can also be derived directly from the equation

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta H[\eta + \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} . \quad (71)$$

The final equation for the condensate wave function follows from Eq. (66) after averaging it over the space \mathcal{F}_1 . In doing this, we define for the noncondensed particles the normal density matrix

$$\rho_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}) \rangle_{\mathcal{F}_1} , \quad (72)$$

the anomalous density matrix

$$\sigma_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle_{\mathcal{F}_1} , \quad (73)$$

and the related diagonal densities

$$\rho_1(\mathbf{r}) \equiv \rho_1(\mathbf{r}, \mathbf{r}) , \sigma_1(\mathbf{r}) \equiv \sigma_1(\mathbf{r}, \mathbf{r}) . \quad (74)$$

The total particle density is

$$\rho(\mathbf{r}) \equiv |\eta(\mathbf{r})|^2 + \rho_1(\mathbf{r}) . \quad (75)$$

Averaging Eq. (67) gives

$$\langle \hat{X}(\mathbf{r}, \mathbf{r}') \rangle_{\mathcal{F}_1} = \rho_1(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle_{\mathcal{F}_1} . \quad (76)$$

Then from Eq. (66) we obtain

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + U - \mu_0 - \mu \right) \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[\rho(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle_{\mathcal{F}_1} \right] d\mathbf{r}' . \quad (77)$$

This is an exact equation valid for any Bose-condensed system, equilibrium or nonequilibrium, uniform or nonuniform.

For an equilibrium system, the coherent field $\eta(\mathbf{r})$ may be treated as not depending on time. Generally speaking, a stationary solution could depend on time as $\eta(\mathbf{r}, t) \propto \exp(-i\mu'_0 t)$. This, however, would simply lead to a redefinition of the Lagrange multiplier μ_0 . Hence, an equilibrium condensate function can be defined as time independent. In that case, Eq. (77) yields

$$\varepsilon \eta(\mathbf{r}) = \left[-\frac{\nabla^2}{2m} + U(\mathbf{r}) \right] \eta(\mathbf{r}) +$$

$$+ \int \Phi(\mathbf{r} - \mathbf{r}') \left[\rho(\mathbf{r}')\eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}')\eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}')\eta^*(\mathbf{r}') + < \psi_1^\dagger(\mathbf{r}')\psi_1(\mathbf{r}')\psi_1(\mathbf{r}) >_{\mathcal{F}_1} \right] d\mathbf{r}' , \quad (78)$$

where the notation

$$\varepsilon \equiv \mu_0 + \mu \quad (79)$$

is introduced, playing the role of the condensate energy per particle. Equation (78) is a generalized eigenproblem, which can possess the whole spectrum of the energies ε and the related eigenfunctions $\eta(\mathbf{r})$. In the case of a confining potential $U(\mathbf{r})$, representing an atomic trap, the spectrum ε is discrete, with the solutions $\eta(\mathbf{r})$ representing topological coherent modes [38–41]. In equilibrium, the lowest-energy mode corresponds to the usual condensate. But in a nonequilibrium system, nonground-state condensates can be generated [38–41].

In a uniform system, where $U(\mathbf{r}) = 0$, we have $\eta(\mathbf{r}) = \eta$, $\rho(\mathbf{r}) = \rho$, with $\rho_1(\mathbf{r}, \mathbf{r}')$ and $\sigma_1(\mathbf{r}, \mathbf{r}')$ depending on the difference $\mathbf{r} - \mathbf{r}'$. Then Eq. (78) reduces to

$$\varepsilon\eta = \rho\Phi_0\eta + \int \Phi(\mathbf{r}) \left[\rho_1(\mathbf{r}, 0)\eta + \sigma_1(\mathbf{r}, 0)\eta^* + < \psi_1^\dagger(0)\psi_1(0)\psi_1(\mathbf{r}) >_{\mathcal{F}_1} \right] d\mathbf{r} . \quad (80)$$

Recall that Eqs. (77), (78), and (80) for the corresponding systems are exact, with no approximations involved.

6 Dilute gas

To illustrate the above equations for some particular cases, let us resort to the dilute-gas approximation, when the inequality

$$|\rho a_s^3| \ll 1 \quad (81)$$

is valid, where $\rho \equiv N/V$ is the average density and a_s is the s -wave scattering length. Then the interaction potential can be modelled by the contact form

$$\Phi(\mathbf{r}) = \Phi_0\delta(\mathbf{r}) , \quad (82)$$

with

$$\Phi_0 \equiv \int \Phi(\mathbf{r}) d\mathbf{r} = 4\pi \frac{a_s}{m} .$$

The condensate-function equation (77) becomes

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + U - \varepsilon \right) \eta(\mathbf{r}) + \Phi_0 \left[\rho(\mathbf{r})\eta(\mathbf{r}) + \rho_1(\mathbf{r})\eta(\mathbf{r}) + \sigma_1(\mathbf{r})\eta^*(\mathbf{r}) + < \psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r})\psi_1(\mathbf{r}) > \right] . \quad (83)$$

The equation of motion (70) for the field operator of noncondensed particles takes the form

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_1(\mathbf{r}) + \Phi_0 \left[2|\eta(\mathbf{r})|^2\psi_1(\mathbf{r}) + \eta^2(\mathbf{r})\psi_1^\dagger(\mathbf{r}) + \hat{X}(\mathbf{r}, \mathbf{r}) \right] , \quad (84)$$

where

$$\hat{X}(\mathbf{r}, \mathbf{r}) = 2\psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r})\eta(\mathbf{r}) + \eta^*(\mathbf{r})\psi_1(\mathbf{r})\psi_1(\mathbf{r}) + \psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r})\psi_1(\mathbf{r}) .$$

In Eq. (83) and in what follows, we shall not specify explicitly the Fock spaces over which the averages are to be taken. This makes it possible to simplify the notation and cannot lead to confusion if, by definition, we accept the rule that each average of operators is calculated in that Fock space, where these operators are defined.

Further simplification can be done by employing the Hartree-Fock-Bogolubov (HFB) approximation. Then

$$\langle \psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r})\psi_1(\mathbf{r}) \rangle = 0 .$$

And the condensate-function equation (83) reduces to

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + U - \varepsilon \right) \eta(\mathbf{r}) + \Phi_0 [\rho(\mathbf{r})\eta(\mathbf{r}) + \rho_1(\mathbf{r})\eta(\mathbf{r}) + \sigma_1(\mathbf{r})\eta^*(\mathbf{r})] . \quad (85)$$

If one considers the case, when all particles are condensed, that is, $\rho(\mathbf{r}) = |\eta(\mathbf{r})|^2$ and $\rho_1(\mathbf{r}) = \sigma_1(\mathbf{r}) = 0$, then Eq. (85) simplifies to the equation

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}) = \left[-\frac{\nabla^2}{2m} + U - \varepsilon + \Phi_0 |\eta(\mathbf{r})|^2 \right] \eta(\mathbf{r}) .$$

The latter is what is generally known as the nonlinear Schrödinger equation and in condensed-matter literature as the Gross-Pitaevskii equation.

In the HFB approximation, the terms entering $\hat{X}(\mathbf{r}, \mathbf{r})$ linearize as

$$\psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r}) = \psi_1^\dagger(\mathbf{r}) \langle \psi_1(\mathbf{r}) \rangle + \langle \psi_1^\dagger(\mathbf{r}) \rangle \psi_1(\mathbf{r}) - \langle \psi_1^\dagger(\mathbf{r}) \rangle \langle \psi_1(\mathbf{r}) \rangle = 0$$

and

$$\psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r})\psi_1(\mathbf{r}) = 2\rho_1(\mathbf{r})\psi_1(\mathbf{r}) + \sigma_1(\mathbf{r})\psi_1^\dagger(\mathbf{r}) ,$$

where the conservation condition (39) is taken into account. The linearized Eq. (84) is

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}) = \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_1(\mathbf{r}) + \Phi_0 [2\rho(\mathbf{r})\psi_1(\mathbf{r}) + \sigma(\mathbf{r})\psi_1^\dagger(\mathbf{r})] , \quad (86)$$

where

$$\sigma(\mathbf{r}) \equiv \eta^2(\mathbf{r}) + \sigma_1(\mathbf{r}) . \quad (87)$$

For an equilibrium system, the condensate-function equation (85) becomes

$$\varepsilon \eta = \left[-\frac{\nabla^2}{2m} + U(\mathbf{r}) \right] \eta(\mathbf{r}) + \Phi_0 [\rho(\mathbf{r})\eta(\mathbf{r}) + \rho_1(\mathbf{r})\eta(\mathbf{r}) + \sigma_1(\mathbf{r})\eta^*(\mathbf{r})] . \quad (88)$$

In the case of a uniform system, when $U(\mathbf{r}) = 0$, the condensate amplitude η can be chosen real. From Eq. (88), taking into consideration that $\rho_1(\mathbf{r}) = \rho_1$ and $\sigma_1(\mathbf{r}) = \sigma_1$, we have

$$\varepsilon = (\rho + \rho_1 + \sigma_1)\Phi_0 . \quad (89)$$

Let us consider in more detail an equilibrium uniform system. The field operator of noncondensed particles can be expanded over the basis of plane waves

$$\varphi_k(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

as

$$\psi_1(\mathbf{r}) = \sum_{k \neq 0} a_k \varphi_k(\mathbf{r}) . \quad (90)$$

Because of the global symmetry of the Hamiltonian with respect to the transformation

$$\eta(\mathbf{r}) \longrightarrow \eta(\mathbf{r}) e^{i\alpha} , \quad \psi_1(\mathbf{r}) \longrightarrow \psi_1(\mathbf{r}) e^{i\alpha} , \quad (91)$$

in which α is a real number, the condensate amplitude $\eta(\mathbf{r}) = \eta$ can be taken real,

$$\eta = \eta^* = \sqrt{\rho_0} , \quad \rho_0 \equiv \frac{N_0}{V} . \quad (92)$$

The field operators a_k and a_k^\dagger in the momentum representation are defined on the Fock space $\mathcal{F}(a_k)$ generated by a_k^\dagger . An important role is played by the following averages. The momentum distribution of particles

$$n_k \equiv \langle a_k^\dagger a_k \rangle \quad (93)$$

is called the normal average, as opposed to

$$\sigma_k \equiv \langle a_k a_{-k} \rangle , \quad (94)$$

termed the anomalous average. The latter gives the amplitude of the process, when two particles are annihilated from the thermal cloud of noncondensed particles. Respectively, $\sigma_k^* = \langle a_k^\dagger a_{-k}^\dagger \rangle$ is the amplitude for the process of creation of two noncondensed particles. With σ_k being the amplitude of these pair processes of creation and annihilation, the absolute value $|\sigma_k|$ describes the density of binary correlated particles.

The averages (93) and (94) define the density of noncondensed particles,

$$\rho_1 \equiv \langle \psi_1^\dagger(\mathbf{r}) \psi_1(\mathbf{r}) \rangle = \frac{1}{V} \sum_{k \neq 0} n_k , \quad (95)$$

and the amplitude of binary correlated particles,

$$\sigma_1 \equiv \langle \psi_1(\mathbf{r}) \psi_1(\mathbf{r}) \rangle = \frac{1}{V} \sum_{k \neq 0} \sigma_k . \quad (96)$$

The total number of noncondensed particles is

$$N_1 = \sum_{k \neq 0} n_k \quad (97)$$

and the number of binary correlated particles is

$$B_1 = \left| \sum_{k \neq 0} \sigma_k \right| . \quad (98)$$

So that the number of correlated pairs is $B_1/2$.

Substituting the field-operator expansion (90) into the Hamiltonian (58), we take the coherent average, as a result of which the condensate operators $\psi_0(\mathbf{r})$ are replaced by the coherent field $\eta(\mathbf{r})$. For the considered uniform system, we find the zero-order term

$$H^{(0)} = \left(\frac{1}{2} \rho_0 \Phi_0 - \varepsilon \right) N_0 . \quad (99)$$

The first-order term $H^{(1)}$ is exactly zero. The second-order term is

$$H^{(2)} = \sum_{k \neq 0} \left(\frac{k^2}{2m} + 2\rho_0 \Phi_0 - \mu \right) a_k^\dagger a_k + \frac{1}{2} \rho_0 \Phi_0 \sum_{k \neq 0} \left(a_k^\dagger a_{-k}^\dagger + a_{-k} a_k \right) . \quad (100)$$

The sum of Eqs. (99) and (100) corresponds to the Hamiltonian in the Bogolubov approximation [7–10]. For the higher-order terms, we obtain the following. The third-order term is

$$H^{(3)} = \sqrt{\frac{\rho_0}{V}} \Phi_0 \sum'_{k,p} \left(a_k^\dagger a_{k+p} a_{-p} + a_{-p}^\dagger a_{k+p}^\dagger a_k \right) , \quad (101)$$

where the prime at the summation sign indicates that no operator in the summation corresponds to a_0 , so that here

$$\mathbf{k} \neq 0 , \quad \mathbf{p} \neq 0 , \quad \mathbf{k} + \mathbf{p} \neq 0 .$$

For the fourth-order term, we get

$$H^{(4)} = \frac{\Phi_0}{2V} \sum_k \sum'_{p,q} a_p^\dagger a_q^\dagger a_{k+p} a_{q-k} , \quad (102)$$

where the prime again means the same as earlier, that is, here it implies that

$$\mathbf{p} \neq 0 , \quad \mathbf{q} \neq 0 , \quad \mathbf{k} + \mathbf{p} \neq 0 , \quad \mathbf{q} - \mathbf{k} \neq 0 .$$

The higher-order terms (101) and (102) can be treated in the HFB approximation. In so doing, we keep in mind that, as a consequence of the conservation condition (39), we have

$$\langle a_k \rangle = 0 \quad (\mathbf{k} \neq 0) . \quad (103)$$

Therefore Eq. (101) vanishes,

$$H^{(3)} = 0 . \quad (104)$$

And Eq. (102) reduces to

$$H^{(4)} = \Phi_0 \sum_{k \neq 0} \left(2\rho_1 a_k^\dagger a_k + \frac{1}{2} \sigma_1 a_k^\dagger a_{-k}^\dagger + \frac{1}{2} \sigma_1^* a_{-k} a_k \right) - \frac{1}{2} (2\rho_1^2 + |\sigma_1|^2) \Phi_0 V . \quad (105)$$

In this way, instead of the Hamiltonian (58), we have in the HFB approximation

$$H_{HFB} = H^{(0)} + H^{(2)} + H^{(4)} , \quad (106)$$

where $H^{(0)}$ is given by Eq. (99); $H^{(2)}$, by Eq. (100); and $H^{(4)}$, by Eq. (105). To write down the Hamiltonian (106) in a compact form, let us introduce the notation

$$\omega_k \equiv \frac{k^2}{2m} + 2\rho\Phi_0 - \mu \quad (107)$$

and, assuming that σ_1 is real, we define

$$\Delta \equiv (\rho_0 + \sigma_1)\Phi_0 . \quad (108)$$

Then Hamiltonian (106) writes as

$$H_{HFB} = E_{HFB} + \sum_{k \neq 0} \omega_k a_k^\dagger a_k + \frac{1}{2} \Delta \sum_{k \neq 0} (a_k^\dagger a_{-k}^\dagger + a_{-k} a_k) , \quad (109)$$

with the HFB nonoperator term

$$E_{HFB} \equiv H^{(0)} - \frac{1}{2} (2\rho_1^2 + \sigma_1^2) \Phi_0 V .$$

Invoking the Bogolubov canonical transformation (21), discussed in Section 3, Hamiltonian (109) is diagonalized to the Bogolubov form

$$H_B = E_0 + \sum_{k \neq 0} \varepsilon_k b_k^\dagger b_k , \quad (110)$$

with the ground-state energy

$$E_0 = E_{HFB} + \frac{1}{2} \sum_{k \neq 0} (\varepsilon_k - \omega_k)$$

and with the spectrum

$$\varepsilon_k = \sqrt{\omega_k^2 - \Delta^2} . \quad (111)$$

Separation of Bose-Einstein condensate by means of the Bogolubov shift is meaningful only when the momentum distribution of particles displays a singularity at the point $k = 0$, which happens if the quasiparticle spectrum, being positive, touches zero at zero momentum [42]. That is, the necessary condition for the occurrence of Bose-Einstein condensation is

$$\lim_{k \rightarrow 0} \varepsilon_k = 0 , \quad \varepsilon_k \geq 0 . \quad (112)$$

This defines the chemical potential

$$\mu = 2\rho\Phi_0 - \Delta ,$$

which, with Eq. (108), becomes

$$\mu = (\rho + \rho_1 - \sigma_1)\Phi_0 . \quad (113)$$

Combining this with Eqs. (79) and (89), we get

$$\mu_0 = \varepsilon - \mu = 2\sigma_1\Phi_0 . \quad (114)$$

Substituting Eq. (113) into Eq. (107), we have

$$\omega_k = \frac{k^2}{2m} + (\rho_0 + \sigma_1)\Phi_0 ,$$

which, taking into consideration Eqs. (108) and (111), can be written as

$$\omega_k = \frac{k^2}{2m} + \Delta = \sqrt{\varepsilon_k^2 + \Delta^2} .$$

The quasiparticle spectrum (111) can be represented in the standard form of the Bogolubov spectrum

$$\varepsilon_k = \sqrt{(ck)^2 + \left(\frac{k^2}{2m}\right)^2} , \quad (115)$$

with the sound velocity given by the equation

$$c \equiv \sqrt{\frac{\Delta}{m}} \quad (\Delta = mc^2) . \quad (116)$$

As is evident, spectrum (115) is gapless, in agreement with the theorems by Bogolubov [9,10] and Hugenholtz and Pines [14]. At the same time, we have encountered no contradiction with the equations of motion. Recall that the latter were derived from one given Hamiltonian, because of which these equations automatically preserve all conservation laws.

The diagonal Hamiltonian (110) makes it easy to calculate different averages in the space $\mathcal{F}(b_k)$. Thus, the momentum distribution of quasiparticles is

$$\pi_k \equiv \langle b_k^\dagger b_k \rangle = (e^{\beta\varepsilon_k} - 1)^{-1} . \quad (117)$$

Taking into account that

$$1 + 2\pi_k = \coth\left(\frac{\beta\varepsilon_k}{2}\right) ,$$

we find the momentum distribution of particles (93) as

$$n_k = \frac{\sqrt{\varepsilon_k^2 + \Delta^2}}{2\varepsilon_k} \coth\left(\frac{\beta\varepsilon_k}{2}\right) - \frac{1}{2} \quad (118)$$

and the anomalous average (94) as

$$\sigma_k = -\frac{\Delta}{2\varepsilon_k} \coth\left(\frac{\beta\varepsilon_k}{2}\right) . \quad (119)$$

For the density of noncondensed particles (95), we obtain

$$\rho_1 = \frac{1}{2} \int \left[\frac{\sqrt{\varepsilon_k^2 + \Delta^2}}{\varepsilon_k} \coth\left(\frac{\beta\varepsilon_k}{2}\right) - 1 \right] \frac{d\mathbf{k}}{(2\pi)^3} , \quad (120)$$

and for the anomalous amplitude (98), we find

$$\sigma_1 = -(\rho_0 + \sigma_1) \int \frac{\Phi_0}{2\varepsilon_k} \coth\left(\frac{\beta\varepsilon_k}{2}\right) \frac{d\mathbf{k}}{(2\pi)^3} . \quad (121)$$

In agreement with the earlier assumption, the amplitude σ_1 can be chosen to be real. However, the integral in Eq. (121) displays an ultraviolet divergence caused by the dilute-gas approximation with the contact potential (82). This artificial divergence can be easily removed by accepting a more realistic interaction potential $\Phi(\mathbf{r})$ possessing a nontrivial momentum dependence of its Fourier transform Φ_k . One often takes the potential $\Phi(\mathbf{r})$ in the Gaussian form [43–45], for which Φ_k exponentially decreases as $k \rightarrow \infty$. Replacing in Eq. (108) Φ_0 by Φ_k , we get

$$\Delta_k \equiv (\rho_0 + \sigma_1)\Phi_k . \quad (122)$$

Now, the integral in Eq. (121) becomes

$$\alpha \equiv \int \frac{\Phi_k}{2\varepsilon_k} \coth\left(\frac{\beta\varepsilon_k}{2}\right) \frac{d\mathbf{k}}{(2\pi)^3} . \quad (123)$$

The latter is convergent as soon as Φ_k tends to zero faster than $1/k^2$.

Another possibility of removing the ultraviolet divergence could be by subtracting the divergent term in Eq. (121), as is often done when considering hard-core particles. In such a manner, integral (123) could be defined as

$$\alpha = \int \left(\frac{\Phi_0}{2\varepsilon_k} - \frac{m\Phi_0}{k^2} \right) \coth\left(\frac{\beta\varepsilon_k}{2}\right) \frac{d\mathbf{k}}{(2\pi)^3} .$$

Note, however, that the latter expression becomes negative, since $\varepsilon_k > k^2/2m$, while Eq. (123) is positive.

Using notation (123), we obtain, instead of Eq. (121), the relation

$$\sigma_1 = -(\rho_0 + \sigma_1)\alpha .$$

Solving the latter, we find

$$\sigma_1 = -\frac{\rho_0\alpha}{1+\alpha} . \quad (124)$$

Because integral (123) is positive, the anomalous amplitude (124) is negative. From Eq. (122), we have

$$\Delta_k = \frac{\rho_0\Phi_k}{1+\alpha} , \quad (125)$$

which is positive for all k . As is seen from Eqs. (124) and (125), in vicinity of the condensation temperature T_c , defined by the equation $\rho_1(T_c) = \rho$, one has $\rho_0 \rightarrow 0$ as $T \rightarrow T_c$. Hence both σ_1 and Δ_k tend to zero when $T \rightarrow T_c$. But for lower temperatures $T \ll T_c$, where ρ_0 can be close to ρ , the anomalous amplitude σ_1 becomes of the order of ρ_1 and can even be much larger than the latter. Therefore the anomalous averages cannot be neglected at low temperatures.

It is necessary to stress the difference between the theory, developed in this paper, and the standard approach to Bose-condensed systems. The principal difference is that in the

present theory two Lagrange multipliers, μ_0 and μ , are introduced in Eq. (57) in order to preserve two normalization conditions (45) and (55). While in the standard theory, solely the chemical potential μ is introduced. because of this, the HFB approximation in the standard theory acquires an unphysical gap in the spectrum of collective excitations. If one removes the gap by some additional tricks, the theory becomes nonconserving. Thus, the standard approach always suffers from one of the deficiencies, being either gapeful or nonconserving [15].

Sometimes, to remove the gap in the collective spectrum, one sets to zero the anomalous average (119), ascribing this trick to Popov. First of all, such a trick is principally incorrect at low temperatures, when the anomalous averages become of the order or larger than the normal averages [46]. And, moreover, as is easy to infer from the original works by Popov [16–19], he has never suggested to use such an incorrect trick at low temperatures.

In the theory, presented in this paper, there is no need to invoke any unjustified tricks. All averages, normal as well as anomalous, are treated on an equal footing. And the theory always remains both gapless and conserving.

In conclusion to this section, it is useful to analyse the stability of matter in the HFB approximation. As is well known [47], the ideal uniform Bose-condensed gas is unstable. This instability stems from the divergent compressibility, which is directly related to anomalous particle fluctuations [5].

There have been published quite a number of papers claiming that particle fluctuations in the interacting Bose gas remain anomalous, being proportional to $N^{4/3}$ in the Bogolubov approximation. This type of anomalous behaviour does not depend on the ensemble employed, being the same in the grand canonical and canonical Gibbs ensembles, as well as in the microcanonical ensemble [48]. If such anomalous fluctuations would really be present, this would mean the instability of the system [5,49,50].

However, as has been thoroughly explained in Ref. [5,49,50], there are no anomalous fluctuations in the Bogolubov approximation. Particle fluctuations in the Bogolubov theory are normal, being proportional to N . The anomalies in the fluctuations arise solely to the unjustified usage of an approximation outside of the region of its validity [49,50].

Let us consider particle fluctuations in the HFB approximation. These fluctuations are characterized by the dispersion

$$\Delta^2(\hat{N}) \equiv \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 . \quad (126)$$

A convenient expression for this dispersion is given [5,49] by the equation

$$\Delta^2(\hat{N}) = N \left\{ 1 + \rho \int [g(\mathbf{r}) - 1] d\mathbf{r} \right\} , \quad (127)$$

in which the pair correlation function

$$g(\mathbf{r}) \equiv \frac{1}{\rho^2} \langle \tilde{\psi}^\dagger(\mathbf{r}) \tilde{\psi}^\dagger(0) \tilde{\psi}(0) \tilde{\psi}(\mathbf{r}) \rangle \quad (128)$$

is defined through the field operators (42).

Calculating function (128), we should keep in mind that the HFB approximation is equivalent to an effective mean-field theory, with a quadratic Hamiltonian in terms of the

field operators $\psi_1(\mathbf{r})$. Therefore, substituting the representation (42) into Eq. (128), we should retain there only the terms up to the second order with respect to $\psi_1(\mathbf{r})$. Then we have

$$g(\mathbf{r}) = 1 + \frac{2\rho_0}{\rho^2} [\rho_1(\mathbf{r}, 0) + \sigma_1(\mathbf{r}, 0)] .$$

Because of the same reason, we should set here $\rho_0/\rho \rightarrow 1$, since $\rho_0 \equiv \rho - \rho_1$. Thus, we get

$$g(\mathbf{r}) = 1 + \frac{2}{\rho} \int (n_k + \sigma_k) e^{i\mathbf{k}\cdot\mathbf{r}} \frac{d\mathbf{k}}{(2\pi)^3} . \quad (129)$$

Using the expressions for n_k and σ_k , obtained above, we find

$$\Delta^2(\hat{N}) = \frac{TN}{mc^2} . \quad (130)$$

That is, particle fluctuations in the HFB approximation are normal, in the same way as in the Bogolubov approximation [5,49,50].

7 Nonuniform matter

The consideration of the previous Section 6 can be generalized to the case of nonuniform Bose systems with arbitrary interaction potentials $\Phi(\mathbf{r})$. As is shown in Section 5, the final equations of motion can be derived by projecting the Hamiltonian (58) on the space \mathcal{F}_1 . This implies that the coherent average of Eq. (58) is taken in the space \mathcal{F}_0 , which results in the replacement of the condensate field operators $\psi_0(\mathbf{r})$ by the condensate wave function $\eta(\mathbf{r})$. Keeping this projection in mind, we shall work now directly in the space \mathcal{F}_1 .

For concreteness, we shall employ the HFB approximation, which for the fourth-order product of the noncondensed-particle field operators writes as

$$\begin{aligned} \psi_1^\dagger(\mathbf{r})\psi_1^\dagger(\mathbf{r}')\psi_1(\mathbf{r}')\psi_1(\mathbf{r}) &= \rho_1(\mathbf{r})\psi_1^\dagger(\mathbf{r}')\psi_1(\mathbf{r}') + \rho_1(\mathbf{r}')\psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r}) + \\ &+ \rho_1(\mathbf{r}', \mathbf{r})\psi_1^\dagger(\mathbf{r}')\psi_1(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}')\psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r}') + \\ &+ \sigma_1(\mathbf{r}, \mathbf{r}')\psi_1^\dagger(\mathbf{r})\psi_1^\dagger(\mathbf{r}') + \sigma_1^*(\mathbf{r}', \mathbf{r})\psi_1(\mathbf{r}')\psi_1(\mathbf{r}) - \rho_1(\mathbf{r})\rho_1(\mathbf{r}') - |\rho_1(\mathbf{r}, \mathbf{r}')|^2 - |\sigma_1(\mathbf{r}, \mathbf{r}')|^2 , \end{aligned} \quad (131)$$

where the notation from Eqs. (72) to (74) is used. Then, instead of Eq. (109), we come to the HFB Hamiltonian for nonuniform matter

$$\begin{aligned} H_{HFB} &= E_{HFB} + \int \psi_1^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U - \mu \right) \psi_1(\mathbf{r}) d\mathbf{r} + \int \Phi(\mathbf{r} - \mathbf{r}') \left[\rho_1(\mathbf{r}')\psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r}) + \right. \\ &+ \rho(\mathbf{r}', \mathbf{r})\psi_1^\dagger(\mathbf{r}')\psi_1(\mathbf{r}) + \frac{1}{2} \sigma(\mathbf{r}, \mathbf{r}')\psi_1^\dagger(\mathbf{r}')\psi_1^\dagger(\mathbf{r}) + \frac{1}{2} \sigma^*(\mathbf{r}, \mathbf{r}')\psi_1(\mathbf{r}')\psi_1(\mathbf{r}) \left. \right] d\mathbf{r}d\mathbf{r}' , \end{aligned} \quad (132)$$

in which the notation

$$\rho(\mathbf{r}, \mathbf{r}') \equiv \eta(\mathbf{r})\eta^*(\mathbf{r}') + \rho_1(\mathbf{r}, \mathbf{r}') \quad (133)$$

and

$$\sigma(\mathbf{r}, \mathbf{r}') \equiv \eta(\mathbf{r})\eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \quad (134)$$

is introduced and where

$$E_{HFB} \equiv H^{(0)} - \frac{1}{2} \int \Phi(\mathbf{r} - \mathbf{r}') \left[\rho_1(\mathbf{r})\rho_1(\mathbf{r}') + |\rho_1(\mathbf{r}, \mathbf{r}')|^2 + |\sigma_1(\mathbf{r}, \mathbf{r}')|^2 \right] d\mathbf{r}d\mathbf{r}' , \quad (135)$$

with $H^{(0)}$ given in Eq. (99).

The quadratic form (132) can be diagonalized by means of the general canonical transformations [20]. For this purpose, we may expand the operators $\psi_1(\mathbf{r})$ and $\psi_1^\dagger(\mathbf{r})$ as

$$\begin{aligned} \psi_1(\mathbf{r}) &= \sum_k \left[u_k(\mathbf{r})b_k + v_k^*(\mathbf{r})b_k^\dagger \right] , \\ \psi_1^\dagger(\mathbf{r}) &= \sum_k \left[u_k^*(\mathbf{r})b_k^\dagger + v_k(\mathbf{r})b_k \right] , \end{aligned} \quad (136)$$

where k is a set of quantum numbers. The transformations, inverse to Eq. (136), are

$$\begin{aligned} b_k &= \int \left[u_k^*(\mathbf{r})\psi_1(\mathbf{r}) - v_k^*(\mathbf{r})\psi_1^\dagger(\mathbf{r}) \right] d\mathbf{r} , \\ b_k^\dagger &= \int \left[u_k(\mathbf{r})\psi_1^\dagger(\mathbf{r}) - v_k(\mathbf{r})\psi_1(\mathbf{r}) \right] d\mathbf{r} . \end{aligned} \quad (137)$$

The operators $\psi_1(\mathbf{r})$ and b_k are assumed to satisfy the Bose commutation relations, which imposes on the coefficient functions $u_k(\mathbf{r})$ and $v_k(\mathbf{r})$ the following restrictions:

$$\begin{aligned} \sum_k [u_k(\mathbf{r})v_k^*(\mathbf{r}') - v_k^*(\mathbf{r})u_k(\mathbf{r}')] &= 0 , \\ \sum_k [u_k(\mathbf{r})u_k^*(\mathbf{r}') - v_k^*(\mathbf{r})v_k(\mathbf{r}')] &= \delta(\mathbf{r} - \mathbf{r}') , \\ \int [u_k(\mathbf{r})v_p(\mathbf{r}) - v_k(\mathbf{r})u_p(\mathbf{r})] d\mathbf{r} &= 0 , \\ \int [u_k^*(\mathbf{r})u_p(\mathbf{r}) - v_k^*(\mathbf{r})v_p(\mathbf{r})] d\mathbf{r} &= \delta_{kp} . \end{aligned} \quad (138)$$

Let us define

$$\omega(\mathbf{r}, \mathbf{r}') \equiv \left[-\frac{\nabla^2}{2m} + U(\mathbf{r}) - \mu + \int \Phi(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r}') d\mathbf{r}' \right] \delta(\mathbf{r} - \mathbf{r}') + \Phi(\mathbf{r} - \mathbf{r}')\rho(\mathbf{r}, \mathbf{r}') \quad (139)$$

and

$$\Delta(\mathbf{r}, \mathbf{r}') \equiv \Phi(\mathbf{r} - \mathbf{r}')\sigma(\mathbf{r}, \mathbf{r}') . \quad (140)$$

Then the diagonalization condition can be represented as a system of equations

$$\begin{aligned} \int [\omega(\mathbf{r}, \mathbf{r}')u_k(\mathbf{r}') + \Delta(\mathbf{r}, \mathbf{r}')v_k(\mathbf{r}')] d\mathbf{r}' &= \varepsilon_k u_k(\mathbf{r}) , \\ \int [\omega^*(\mathbf{r}, \mathbf{r}')v_k(\mathbf{r}') + \Delta^*(\mathbf{r}, \mathbf{r}')u_k(\mathbf{r}')] d\mathbf{r}' &= -\varepsilon_k v_k(\mathbf{r}) , \end{aligned} \quad (141)$$

which is a variant of the Bogolubov - de Gennes equations. The HFB Hamiltonian (132) acquires the diagonal form

$$H_B = E_0 + \sum_k \varepsilon_k b_k^\dagger b_k , \quad (142)$$

which is analogous to Eq. (110), with the difference that here k is not momentum but a set of quantum numbers labelling the functions $u_k(\mathbf{r})$ and $v_k(\mathbf{r})$. And the ground-state energy is

$$E_0 = E_{HFB} - \sum_k \varepsilon_k \int |v_k(\mathbf{r})|^2 d\mathbf{r} . \quad (143)$$

Calculating the averages in the space $\mathcal{F}(b_k)$, with the Hamiltonian (142), we find the normal density matrix

$$\rho_1(\mathbf{r}, \mathbf{r}') = \sum_k [\pi_k u_k(\mathbf{r}) u_k^*(\mathbf{r}') + (1 + \pi_k) v_k^*(\mathbf{r}) v_k(\mathbf{r}')] \quad (144)$$

and the anomalous density matrix

$$\sigma_1(\mathbf{r}, \mathbf{r}') = \sum_k [\pi_k u_k(\mathbf{r}) v_k^*(\mathbf{r}') + (1 + \pi_k) v_k^*(\mathbf{r}) u_k(\mathbf{r}')] , \quad (145)$$

defined in Eqs. (72) and (73), with π_k from Eq. (117). The corresponding diagonal elements (74) give the density of noncondensed particles

$$\rho_1(\mathbf{r}) = \sum_k [\pi_k |u_k(\mathbf{r})|^2 + (1 + \pi_k) |v_k(\mathbf{r})|^2] \quad (146)$$

and the anomalous amplitude

$$\sigma_1(\mathbf{r}) = \sum_k (1 + 2\pi_k) u_k(\mathbf{r}) v_k^*(\mathbf{r}) . \quad (147)$$

These general equations are valid for an arbitrary external potential $U(\mathbf{r})$ and for any pair interaction potential $\Phi(\mathbf{r})$.

One can always return to the uniform system by taking

$$u_k(\mathbf{r}) = u_k \varphi_k(\mathbf{r}) , \quad v_k(\mathbf{r}) = v_k \varphi_k(\mathbf{r}) , \quad (148)$$

where $\varphi_k(\mathbf{r})$ is a plane wave, By expanding in the plane waves the kernel (139) as

$$\omega(\mathbf{r}, \mathbf{r}') = \sum_k \omega_k \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r}') \quad (149)$$

and Eq. (140) as

$$\Delta(\mathbf{r}, \mathbf{r}') = \sum_k \Delta_k \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r}') , \quad (150)$$

we obtain ω_k and Δ_k , which are equivalent to Eqs. (107) and (108), respectively.

In this way, any system with Bose-Einstein condensate can be described by a self-consistent theory, which is both *conserving* and *gapless*. The basis for this theory is an accurate usage of the nonequivalent operator representations, associated with canonical commutation relations, and the derivation of equations of motion taking into consideration all conditions characterizing the Bose-condensed system. In particular, taking into account two normalization conditions (45) and (55) requires to introduce two Lagrange multipliers μ_0 and μ .

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